



Research Article

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## Studies on effective atomic numbers and electron densities of some chemical explosives in the energy range 1KeV – 100 GeV

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### ABSTRACT

The effective atomic numbers and electron densities of few chemical explosives (CW), viz., Trinitrotoluene (TNT), Trinitrophenylmethylnitramine (Tetryl), Pentaerythritoltetranitrate (PETN), Ciklotrimetilentrinitramin (RDX), Picrylchloride (PC), Nitroglycerin (NG) and Octogene (OG) have been calculated for total and partial photon interactions by the direct method in the wide energy range of 1 KeV-100 GeV using WinXCOM. The values of these parameters have been found to change with energy and composition of the chemical explosives (CW). The variations of effective atomic number and electron density with energy are shown graphically for all photon interactions. The variation of photon mass attenuation coefficients with energy are shown graphically only for total photon interaction. The variation of effective atomic number  $Z_{\text{eff}}$  and electron densities  $N_{\text{el}}$  is due to the variations in the dominance of different interaction processes in that particular energy region.

**Keywords:** Chemical explosives; Photon mass attenuation coefficients; Effective atomic numbers; Electron densities.

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### INTRODUCTION

In view of the extensive use of radiative sources in medicine, agriculture, industry, security screening etc., the study of photon-atom interactions (attenuation and energy absorption coefficients) and effective atomic numbers in different materials have gained importance in the recent years. The photon mass attenuation coefficient, effective atomic number and electron density are the basic quantities required in determining the penetration of X-rays and gamma photons in matter.

The mass attenuation coefficient ( $\mu/\rho$ ) is a measure of probability of interaction that occurs between incident photons and matter per unit area. The knowledge of mass attenuation coefficients of X-rays and gamma photons in biological, chemical and other important materials is of significant practical interest for industrial, biological, agricultural, defence and medical applications [1]. Accurate values of photon mass attenuation coefficients are required to provide essential data in diverse fields such as nuclear diagnostics (computerized tomography), nuclear medicine, radiation protection, radiation dosimetry, gamma ray fluorescence studies, radiation physics, shielding, security screening and etc. The mass attenuation coefficients are widely used in the calculation of photon penetration and energy deposition in shielding, biological and other dosimetric materials.

G. J. Hine [2] has pointed out that in composite materials, for photon interactions, a single number cannot represent the atomic number uniquely across the entire energy region, as in the case of pure elements. This number for composite materials is known as "effective atomic number" ( $Z_{\text{eff}}$ ) and it varies with energy. The energy absorption in a given medium can be calculated if certain constants are known. These necessary constants are  $Z_{\text{eff}}$  and electron density  $N_{\text{el}}$  of the medium. As effective atomic numbers and electron densities are useful in many technological applications, several investigators [3-19] have made extensive studies of effective atomic numbers in variety of composite materials like alloys, polymers, compounds, and mixtures, thermoluminescent dosimetric compounds,

semiconductors and superconductors. In the past Hiremath and Chikkur (20) Manjunathaguru and Umesh (21) recently Pravina Pawar and Govind Bichile (22) have reported effective atomic numbers for some chemical compounds containing H, C, O, N atoms.

The effective atomic number  $Z_{\text{eff}}$  has an interesting application which can be used in security screening of air passenger luggage for chemical explosives, in particular for substance of low crystalline (23). There are almost no reports on the effective atomic number and electron density studies of chemical explosives in literature. This prompted us to study the mass attenuation coefficient ( $\mu/\rho$ ) and hence effective atomic number  $Z_{\text{eff}}$  and electron density  $N_{\text{el}}$ . In this paper we report the effective atomic number and electron densities of chemical explosive calculated by using WinXcom program in the energy region 1 KeV-100 GeV.

In today's society acts of terrorism must involve in some stages the illicit trafficking either of explosives, chemical agents, nuclear materials and humans. Therefore the society must rely on the anti trafficking infrastructure. Modern personal, parcel, vehicle and cargo inspection systems are non invasive imaging techniques based on the use of nuclear analytical techniques. The inspection systems are using penetrating radiations (neutrons, gamma and x-ray) in the scanning geometry with the detection of transmitted or radiation produced in the investigated sample.

Explosives and chemical agent's detection systems are based on the fact that the problem of identification can be reduced to the problem of measurement of elemental concentrations. An ever increasing danger of terrorist actions involving theft and unauthorized proliferation of fissionable and radioactive materials make it imperative to develop and manufacture reliable equipment for detection of explosive fissionable and radioactive materials concealed inside various object and luggage. [24]

The first explosive known was gun powder also called black powder. It was the only explosive known for several hundred years' nitrocellulose and nitro glycerine were the first modern explosive. Since then nitrates, nitro compounds fulminates and azides have been the chief explosive compounds used alone or in mixtures with fuels or other agents. Today we have a list of around 100 explosive materials. However, the most often used explosives are trinitrotoluene (TNT), trinitrophenylmethylnitramine (Tetryl), Pentaerythritoltetranitrate (PETN), ciklotrimetilentrinitramin (RDX), Picryl chloride (PC), Nitro-glycerine (NG), and Octogone (OG); their molecular formulae are as shown in table 1.

In the present work, the effective atomic number and electron densities have been calculated for seven chemical explosives for all photon interactions (coherent, incoherent, photoelectric, pair production and total photon interaction [with coherent]) in the energy range 1 KeV - 100 GeV. The variations of effective atomic number and electron density with energy are shown graphically for the all photon interactions. The variations of photon mass attenuation coefficient with energy is also shown graphically only for total photon interaction.

## 2. The method of computation and theoretical basis

A parallel beam of mono energetic X-ray or Gamma photons passing through matter is attenuated due to absorption and scattering. Attenuation due to absorption follows the Beer –Lambert's law,

$$I = I_0 e^{-\mu x} = I_0 e^{-(\mu/\rho)d}, \quad (1)$$

where  $I_0$  and  $I$  are the un-attenuated and attenuated photon intensities,  $d$  is the mass per unit area ( $\text{g}/\text{cm}^2$ ) and  $\mu/\rho$  is the photon mass attenuation coefficient ( $\text{cm}^2/\text{g}$ ). The photon mass attenuation coefficient  $(\mu/\rho)_c$  for any chemical compound or mixture of elements is given by the 'mixture rule' [1]

$$(\mu/\rho)_c = \sum_i w_i (\mu/\rho)_i, \quad (2)$$

where  $w_i$  and  $(\mu/\rho)_i$  are the weight fraction and photon mass attenuation coefficient of the  $i$ th constituent element, respectively. For a chemical compound the fraction by weight ( $w_i$ ) is given by;  $w_i = \frac{n_i A_i}{\sum_j n_j A_j}$ , where  $A_i$  is the atomic weight of the  $i$ th element and  $n_i$  is the number of formula units.

The total cross-section ( $\sigma$ ) in turn can be related as the sum of partial cross sections,

$$\sigma = \sigma_{\text{coh}} + \sigma_{\text{incoh}} + \tau + K + \sigma_{\text{ph, n}}, \quad (3)$$

where  $\sigma_{\text{coh}}$ ,  $\sigma_{\text{incoh}}$ , are coherent (Rayleigh) and incoherent (Compton) scattering cross-sections, respectively.  $\tau$  is the atomic photoelectric cross-section,  $K$  is the positron electron pair production cross section and  $\sigma_{\text{ph, n}}$  is the photonuclear cross –section .

The values of mass attenuation coefficient were then used to determine the total molecular cross-section ( $\sigma_m$ ) by the following relation,

$$\sigma_m = \frac{M}{N_A} \left( \frac{\mu}{\rho} \right)_c, \quad (4)$$

where  $M = \sum_i n_i A_i$  is the molecular weight of the compound,  $N_A$  is the Avogadro's number,  $n_i$  is the total number of atoms (with respect to mass number) in the molecule,  $A_i$  is the atomic weight of  $i$ th element in a molecule.

The effective (average) atomic cross-section ( $\sigma_a$ ) can easily be determined from the following equation,

$$\sigma_a = \frac{1}{N_A} \sum f_i A_i \left( \frac{\mu}{\rho} \right)_i \quad (5)$$

Similarly, effective electronic cross-section ( $\sigma_e$ ) for the individual element is given by the following formula,

$$\sigma_e = \frac{1}{N_A} \sum \frac{f_i A_i}{Z_i} \left( \frac{\mu}{\rho} \right)_i = \frac{\sigma_a}{Z_{eff}}, \quad (6)$$

where  $f_i = n_i / \sum_j n_j$  and  $Z_i$  are the fractional abundance and atomic number of constituent element, respectively.  $n_i$  is the total number of atoms of the constituent element,  $\sum_j n_j$  is the total number of atoms present in the molecular formula.

Now, the effective atomic number ( $Z_{eff}$ ) can be given as  $Z_{eff} = \frac{\sigma_a}{\sigma_e}$  (7)

The effective electron density,  $N_{el}$  (number of electrons per unit mass) can be derived by using Eqs. (2) and (6),

$$N_{el} = \frac{(\mu/\rho)_c}{\sigma_e} = \frac{N_A}{M} Z_{eff} \sum_i n_i \quad (8)$$

Theoretical values for the mass attenuation coefficient can be found in the tabulation by Hubbell and Seltzer [25]. Instead of interpolating tabulated values and using the mixture rule, some computer programs such as WinXCom or its predecessor XCOM can save a lot of manual work and of course time. The XCOM program was originally developed by Berger and Hubbell [26] for calculating mass attenuation coefficients or photon interaction cross-section for any element, compound or mixture in the energy range 1 keV-100 GeV. Later this well-known and widely used program was enhanced and transformed to the Windows platform by Gerward *et al.* [27, 28] under the name WinXCom. All computations in the present work have been carried out using the program WinXCom.

## RESULTS AND DISCUSSION

In the present work, the variations of  $Z_{eff}$  and  $N_{el}$  with photon energy for chemical explosives composed of different elements in different proportions (Table 1) were studied. The results are shown graphically in Figs. 2-13 for partial and total photon interaction processes. The  $Z_{eff}$  and  $N_{el}$  values of chemical explosives are given in Table 2 only for total photon interaction. The present results clearly confirm the comment made by Hine [2] mentioned earlier that the effective atomic number varies with energy. In the following paragraphs energy dependence of  $Z_{eff}$  and  $N_{el}$  for total and individual photon interactions are discussed.

### 3.1. Total photon interaction (with coherent)

Fig. 1 shows the results of total mass attenuation coefficient of chemical explosives against photon energy. From the figure it can be easily seen that (i) there are three energy ranges where photoelectric absorption, Compton scattering and pair production, respectively, are the dominating attenuation processes and (ii) in case of Picryl chloride (PC), there are two values for total mass attenuation coefficients at 2.82 keV due to the chlorine K absorption edge. The value  $1.87 \times 10^2 \text{ cm}^2/\text{g}$  is valid immediately below the absorption edge and the value  $3.96 \times 10^2 \text{ cm}^2/\text{g}$  immediately above absorption edge. It is seen that variation in  $(\mu/\rho)_c$  with chemical composition is large below 100 keV and significant between 0.1- 10 MeV and further there is negligible variation in  $(\mu/\rho)_c$  up to 100 MeV photon energy. These variations are interpreted as being due to (i) photoelectric effect which varies as  $Z^{4-5}$  and (ii) less but significantly due to coherent scattering which varies as  $Z^{2-3}$ . This fact has been verified experimentally by Singh [29] by measuring total mass attenuation coefficient of some soils. The present theoretical results are similar to the observations of Zavel'ski [30] who proposed a direct relation of  $(\mu/\rho)$  with heavy metals in the rock salt at low energy. In the intermediate energy region, where incoherent scattering is the most dominant process, the

mass attenuation coefficient is found to be constant and is due to the linear  $Z$ -dependence of incoherent scattering and insignificant role played by pair production. In the high energy region, the variation in mass attenuation coefficient is due to the  $Z^2$ -dependence of pair production (30).

The variation of  $Z_{\text{eff}}$  with photon energy for total photon interaction (Fig.2) shows the dominance of different interaction process in different energy regions. The behaviour of all chemical explosives is almost identical except Picryl chloride (PC). This is in line with the parthasaradhi [7] who reported that  $Z_{\text{eff}}$  of alloys is different for different interaction processes. Recently similar result was reported by Manohara et al [31] for amino acids.

In low energy region photoelectric interaction is dominant;  $Z_{\text{eff}}$  varies as in case of photo interaction process. From 3-8 keV onwards there is a sharp decrease in  $Z_{\text{eff}}$  with energy up to 150 keV, showing that contribution of scattering processes increases which decreases  $Z_{\text{eff}}$ . This is also confirmed by Sastry and Jayanand [3] who confirmed that  $Z_{\text{eff}}$  of composite material for photoelectric interaction is greater than other processes.

From 150 keV to 3 MeV,  $Z_{\text{eff}}$  is almost independent of energy. This may be due to the dominance of incoherent scattering in this region. From 3 to 400 MeV, there is regular increase in  $Z_{\text{eff}}$  with photon energy. This behaviour is due to mixed contribution of incoherent scattering and pair production. Above 400 MeV,  $Z_{\text{eff}}$  remains almost constant. This may be due to the dominance of pair production in the high energy region. It is observed that the variation in  $Z_{\text{eff}}$  also depends upon relative proportion and the range of atomic numbers of the elements of which chemical explosive is composed (Fig.2). The Picryl chloride (PC) has a large range of  $Z$ 's from 1(H) to 17 (Cl) than any other chemical explosives due to which the variation in its  $Z_{\text{eff}}$  with energy is very significant in comparison to any other chemical explosive, showing jump in low energy region.

### 3.2. Photoelectric absorption

The variation of  $Z_{\text{eff}}$  with photon energy for photoelectric absorption is shown in Fig. 3 which indicates that  $Z_{\text{eff}}$  is almost independent of photon energy for all the chemical explosives except for Picryl chloride (PC). In case of Picryl chloride the sudden jump occurs in  $Z_{\text{eff}}$  at 2.82 keV, which is the K absorption edge energy of chlorine. From 3 keV onwards  $Z_{\text{eff}}$  increases sharply up to 3 MeV and then it remains constant thereafter. This is due to the fact that photoelectric process is predominant at low energies (<1MeV) and for materials of higher atomic numbers than for low  $Z$  materials. Similar results were also obtained by Perumallu et al. [11] in multielement materials of biological importance and Manohara et al. [31] in essential amino acids. This type of  $Z_{\text{eff}}$  variation is probably due to more number of elements present in Picryl chloride (PC) compared to other chemical explosives. These results are in line with the results of Rama Rao et al. [4] and lingam et al. [10]. In all chemical explosives the variation of  $Z_{\text{eff}}$  is almost independent of energy. It is due to the fact that the listed chemical explosives have same elements and are of close atomic number except Picryl chloride.

### 3.3 Incoherent (Compton) scattering

The variation of  $Z_{\text{eff}}$  with photon energy for incoherent scattering is shown in Fig. 4 which indicates that  $Z_{\text{eff}}$  increases sharply with increase in energy in the region 1-200 keV. Beyond 200 keV,  $Z_{\text{eff}}$  is independent of photon energy for all chemical explosives. Most of the elements in a composite material have a value of  $Z/A$  of about 0.5 where as hydrogen has a value of 1.0, which effects Compton scattering. In case of Picryl chloride (PC) the weight percentage of hydrogen is 8.14 which is the lowest among all chemical explosives studied. The present theoretical results are similar to the theoretical results of Manohara et al. [31] and Mudahar et al, [32] who have reported similar types of variations of  $Z_{\text{eff}}$  for alloys and amino acids respectively. The present theoretical results are similar to the experimental findings of Parthasaradhi [9] who has reported the constancy of Compton  $Z_{\text{eff}}$  in the energy range from 100 to 662 keV for some alloys. Khayyoom and parthasarsdhi [9] have studied  $Z_{\text{eff}}$  of some alloys; their experimental result suggests that in incoherent scattering  $Z_{\text{eff}}$  is independent of photon energy from 20 to 800 keV. In our study of chemical explosives,  $Z_{\text{eff}}$  is independent of photon energy only above 200 keV but depends on photon energy below 200 keV. The variation of  $Z_{\text{eff}}$  depends on respective proportion and the range of atomic numbers of the elements of which chemical explosives are composed.

### 3.4 Coherent (Rayleigh) scattering.

The variation of  $Z_{\text{eff}}$  with photon energy for coherent scattering is shown in Fig. 5. From figure it is clear that  $Z_{\text{eff}}$  increases with increase in energy from 1-150 keV (TNT), 1-80 keV (Tetryl), 1-200 keV (PETN and NG) 1-400 keV (RDX), 1-600 keV (PC), 1-100 keV for OG. From the upper limit onwards  $Z_{\text{eff}}$  remains constant with increase in energy i.e. independent of energy. The behaviour of Picryl chloride (PC) is different from other chemical explosive is due to the presence of chlorine (14.32 wt%). El-Kateb and Abdul Hamid [33] have shown that in materials containing carbon, hydrogen, oxygen the effective atomic number tends to be constant as a function of energy. Our results are in good agreement with their results at higher energy but differ slightly at lower energy.

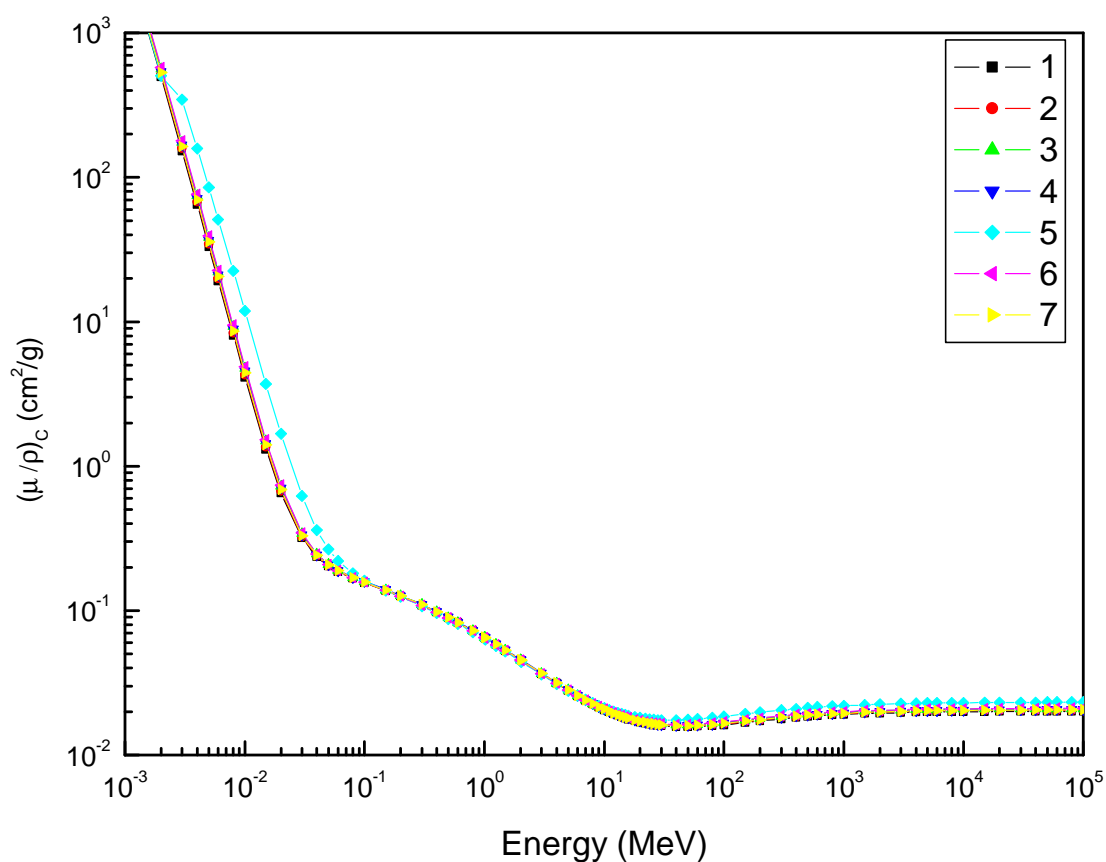
### 3.5 Pair production (nuclear field)

The variation of  $Z_{\text{eff}}$  with photon energy for pair production in nuclear field is shown in Fig. 6, which shows that  $Z_{\text{eff}}$  slightly decreases with increase in photon energy from 1.25 to 2000 MeV and then it is almost independent of energy {except for Picryl chloride(PC)}. It may be due to the fact that pair production in nuclear field is  $Z^2$  dependent. In case of Picryl chloride (PC), below 10 MeV, the fall in  $Z_{\text{eff}}$  with energy is more due to the large range of atomic numbers from 1(H) to 17(Cl).

### 3.6 Pair production (electric field)

The variation of  $Z_{\text{eff}}$  with photon energy for pair production in electric field is shown in Fig. 7. From figure it is clear that  $Z_{\text{eff}}$  is independent of photon energy from 3 keV to ~ 60 MeV. From 60 MeV onwards,  $Z_{\text{eff}}$  decreases with increase of photon energy up to 15 GeV and then it is independent of energy thereafter for all chemical explosives.

The variations of  $N_{\text{el}}$  with photon energy in all the chemical explosives for partial and total interaction processes are similar to that of  $Z_{\text{eff}}$  and can be explained on the similar manner as that of  $Z_{\text{eff}}$  and are shown in Figs.8-13.



**Fig. 1.** Variation of photon mass attenuation coefficient  $(\mu/\rho)_c$  of chemical explosives of Trinitrotoluene (TNT), Trinitrophenylmethylnitramine (Tetryl), Pentaerythritoltetranitrate (PETN), Ciklotrimetilentrinitramin (RDX), Picrylchloride (PC), Nitroglycerin (NG) and Octogene (OG)

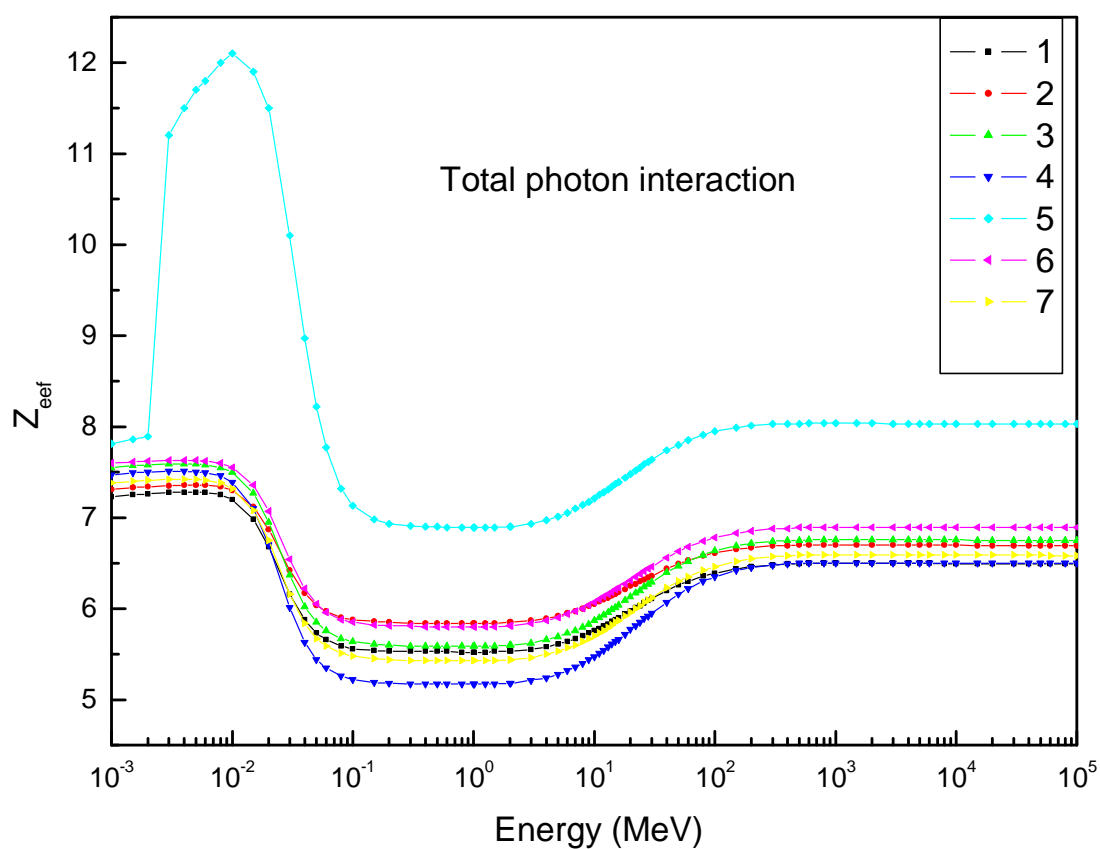


Fig. 2. Variation of effective atomic number  $Z_{\text{eff}}$  of Chemical Explosives with photon energy for total photon interaction (with coherent).

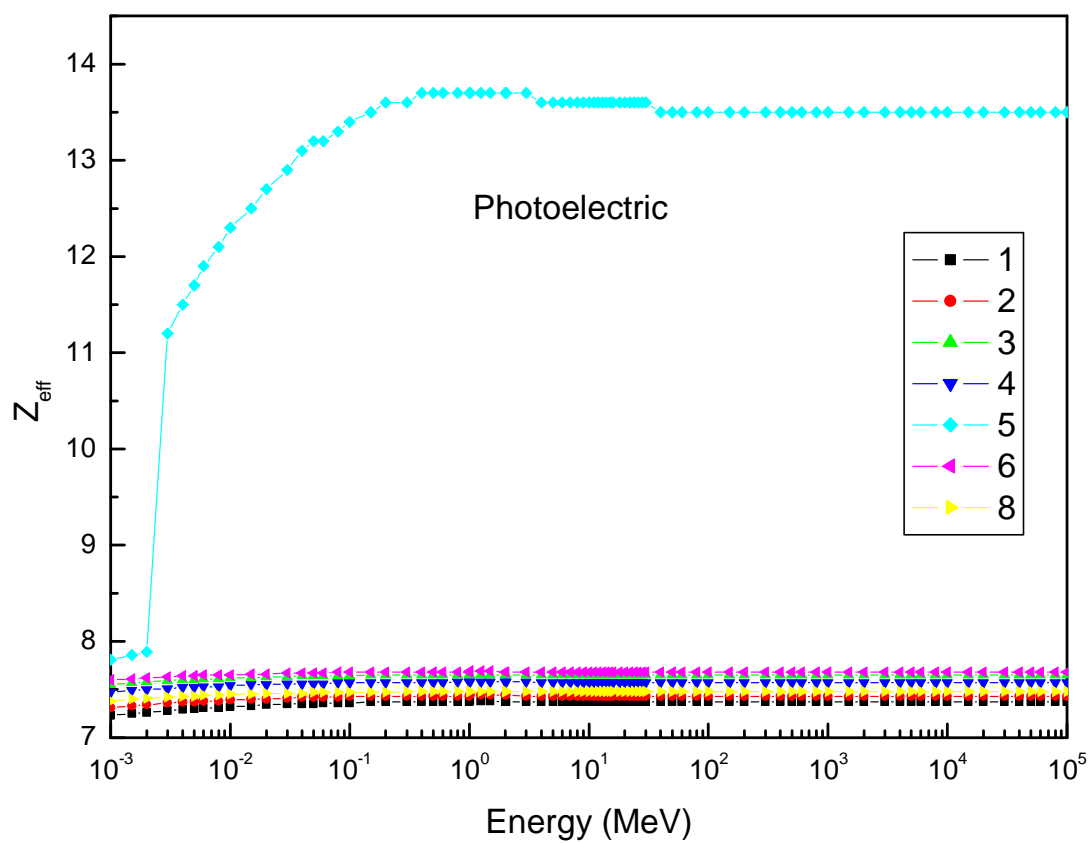


Fig. 3. Variation of effective atomic number  $Z_{\text{eff}}$  of chemical explosives with photon energy for photoelectric absorption.

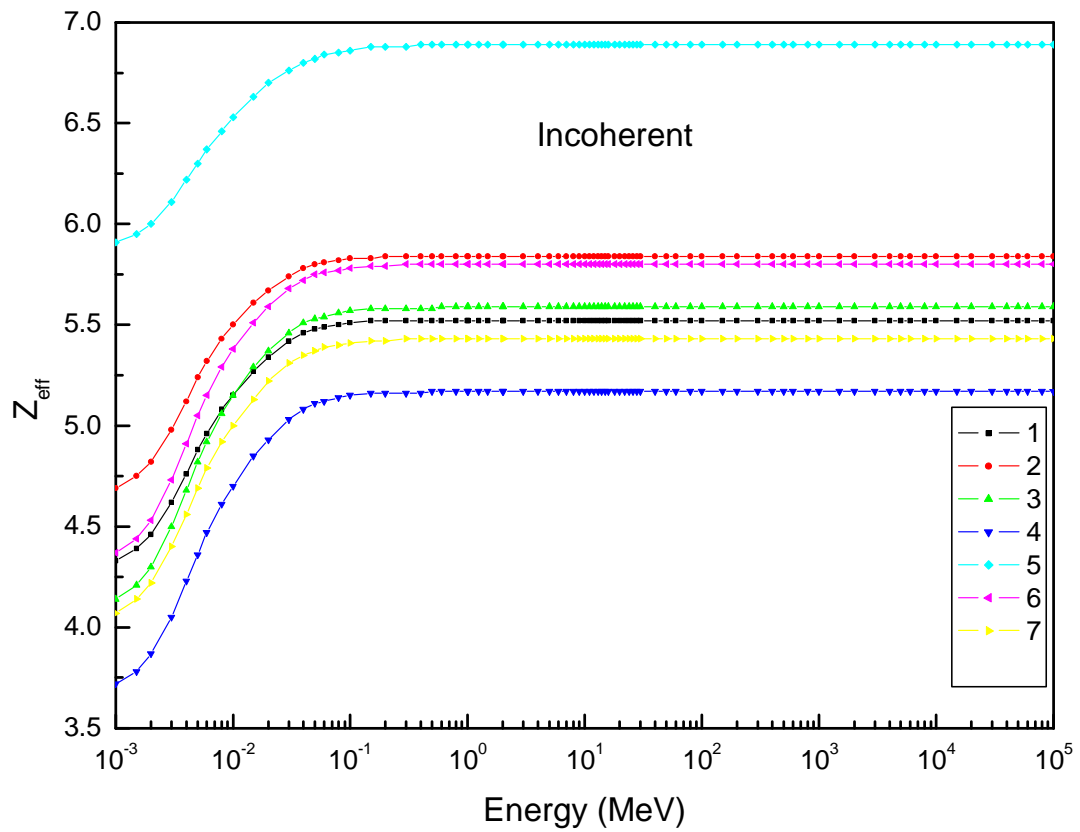


Fig. 4. Variation of effective atomic number  $Z_{\text{eff}}$  of chemical explosives with photon energy for incoherent scattering.



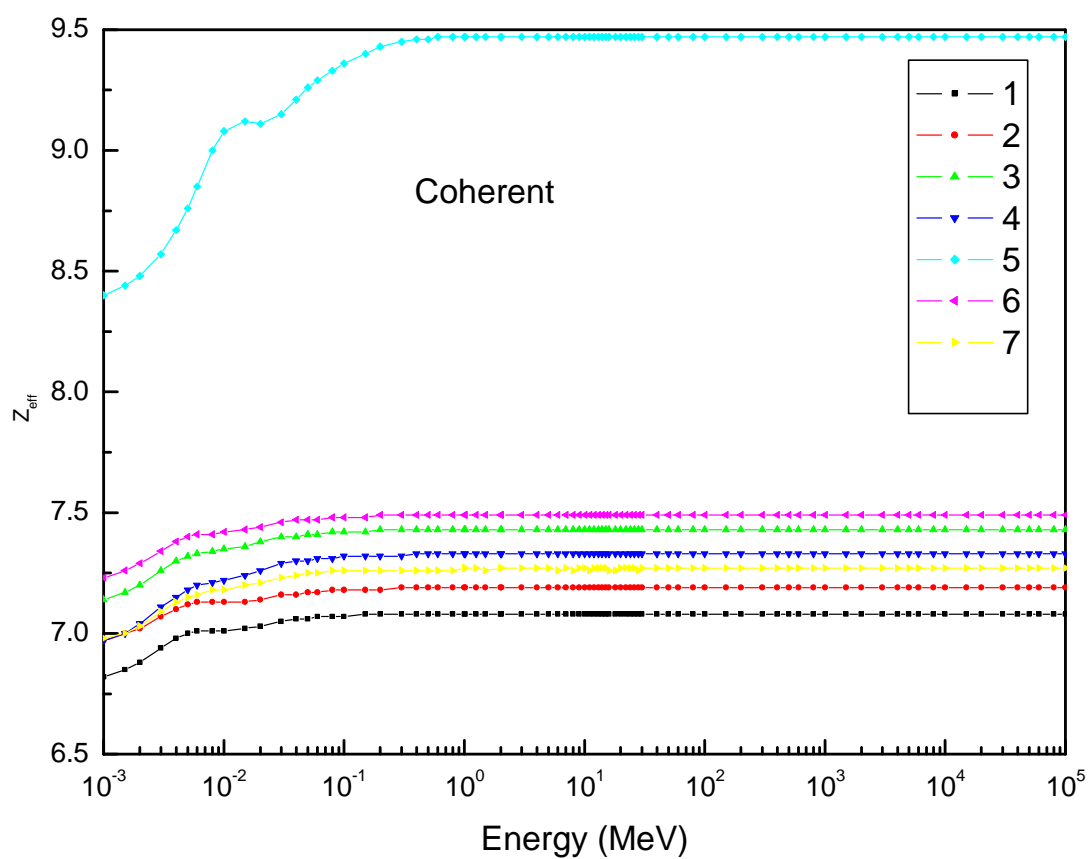


Fig. 5. Variation of effective atomic number  $Z_{\text{eff}}$  of chemical explosives with photon energy for coherent scattering.

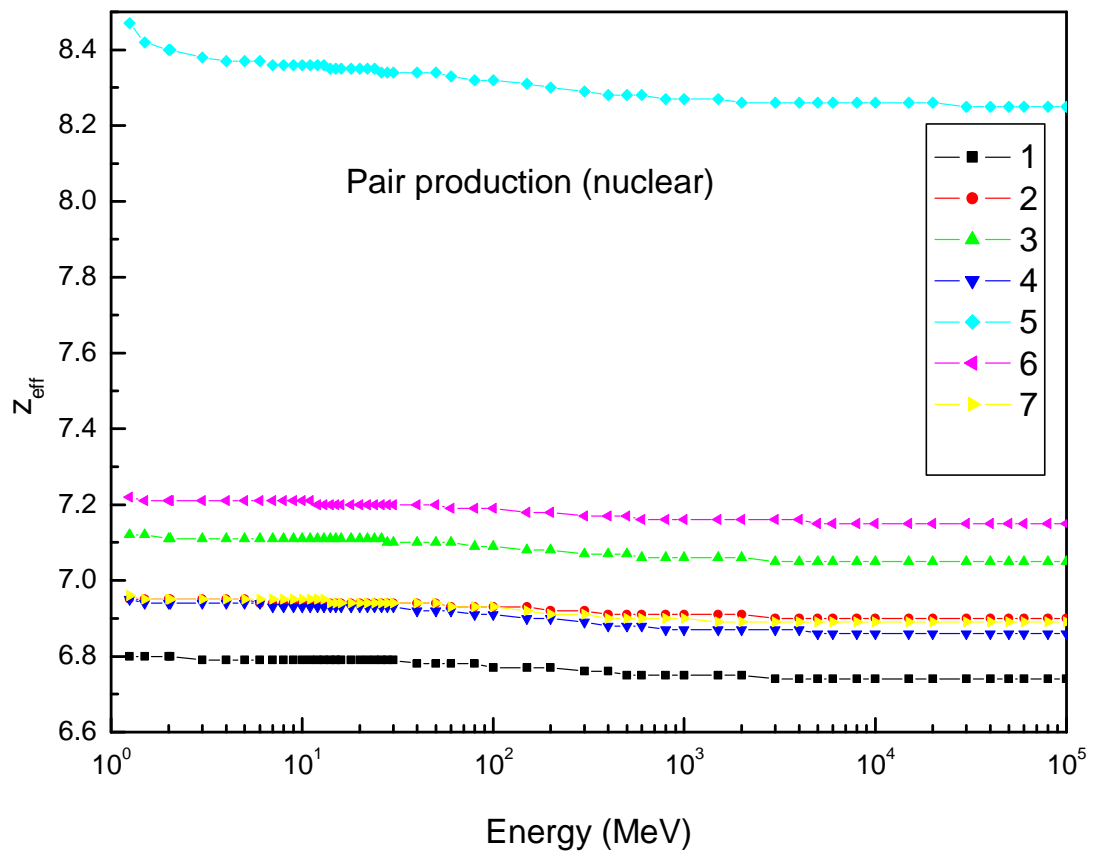


Fig. 6. Variation of effective atomic number  $Z_{\text{eff}}$  of chemical explosives with photon energy for pair production in nuclear field.

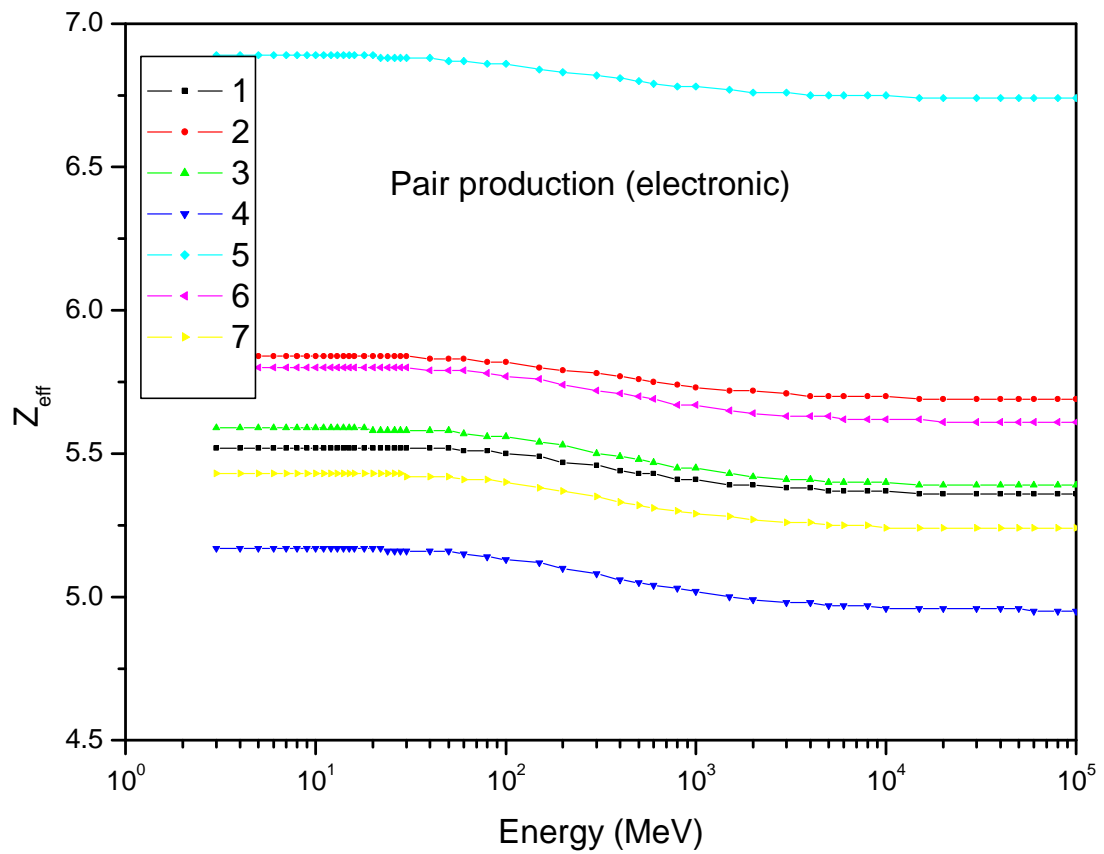


Fig. 7. Variation of effective atomic number  $Z_{\text{eff}}$  of chemical explosives with photon energy for pair production in electric field.

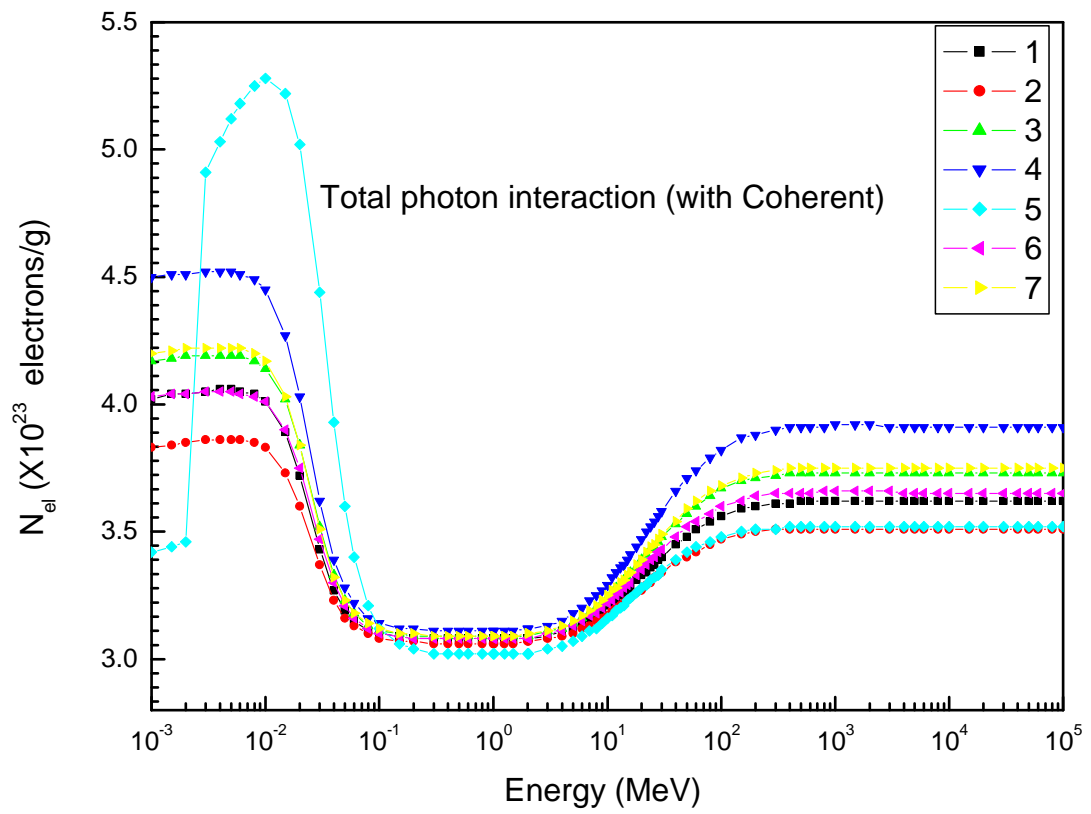


Fig. 8. Variation of effective electron density  $N_{ei}$  of chemical explosives with photon energy for total photon interaction (with coherent)

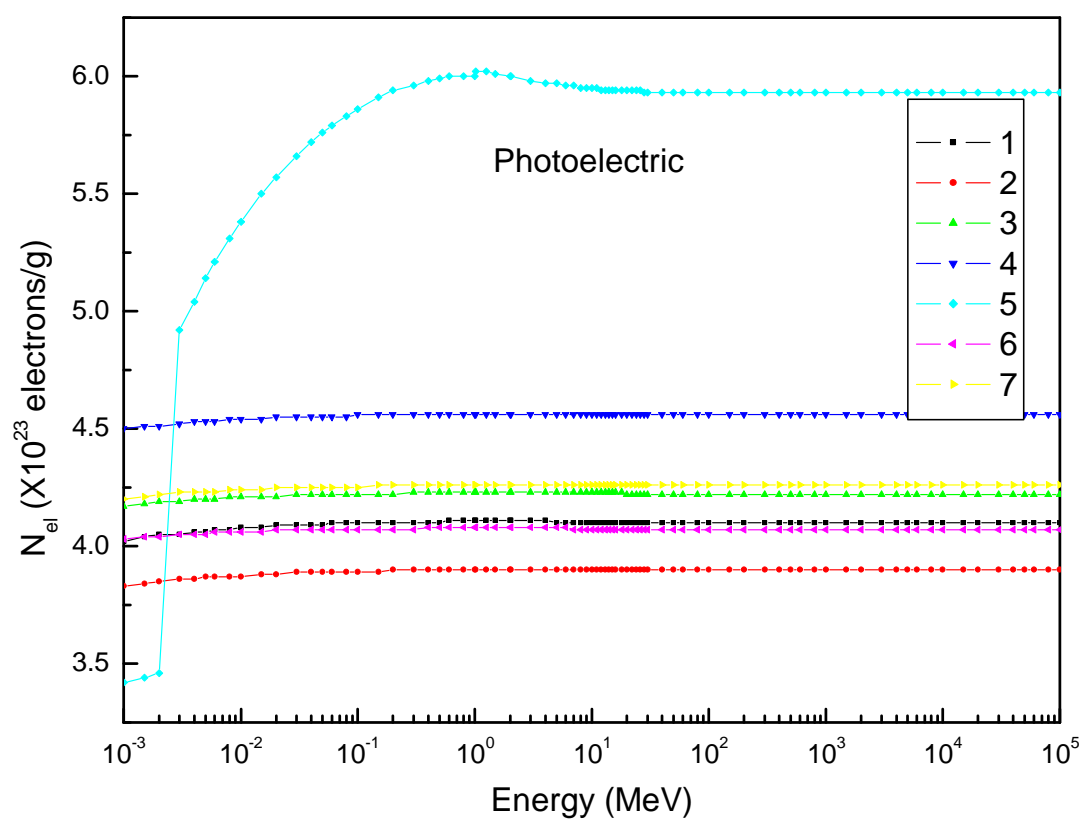


Fig. 9. Variation of effective electron density  $N_{el}$  of chemical explosives with photon energy for photoelectric absorption.

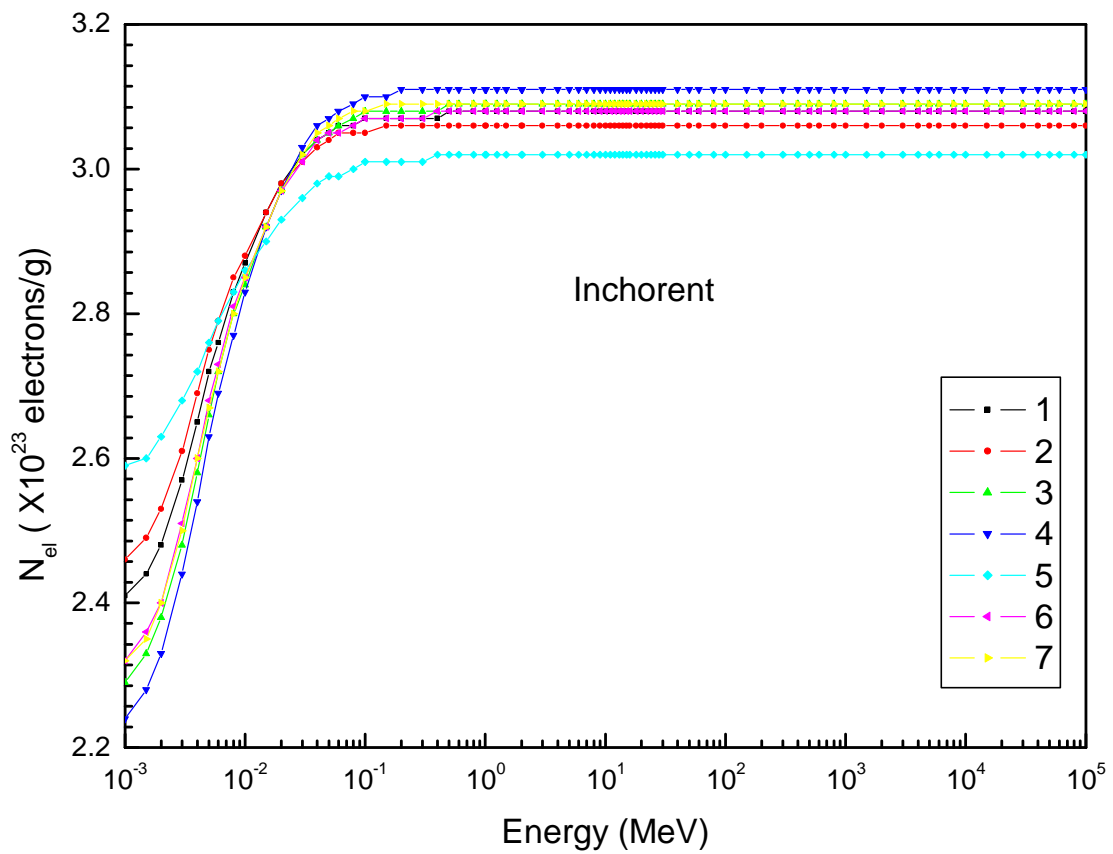


Fig. 10. Variation of effective electron density  $N_{el}$  of chemical explosives with photon energy for incoherent scattering.

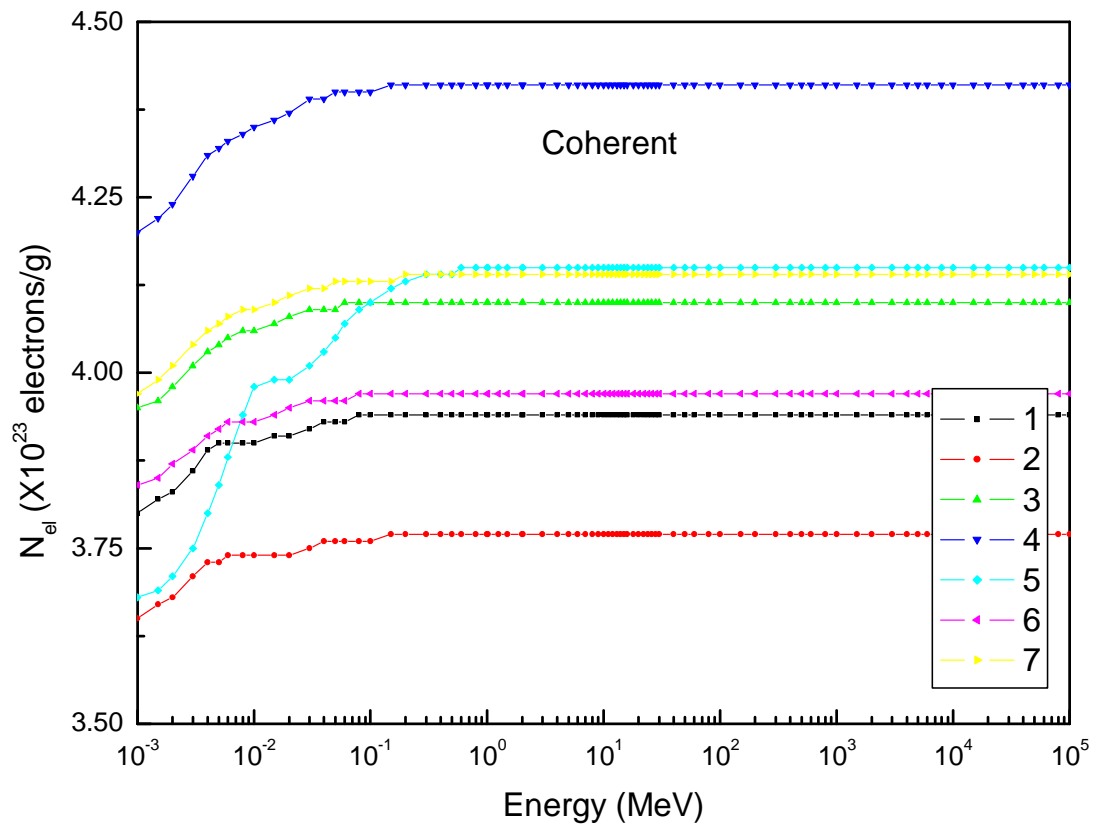


Fig. 11. Variation of effective electron density  $N_{ei}$  of chemical explosives with photon energy for coherent scattering.

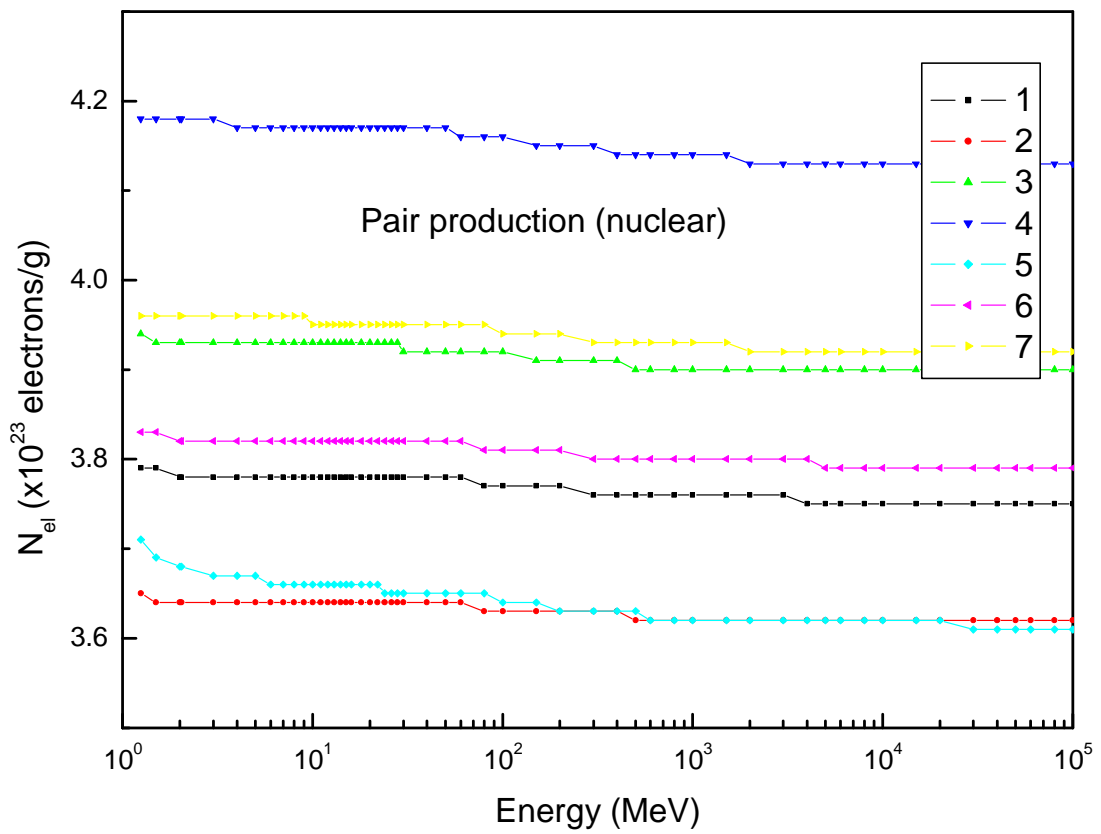


Fig. 12. Variation of effective electron density  $N_{ei}$  of chemical explosives with photon energy for pair production in nuclear field.



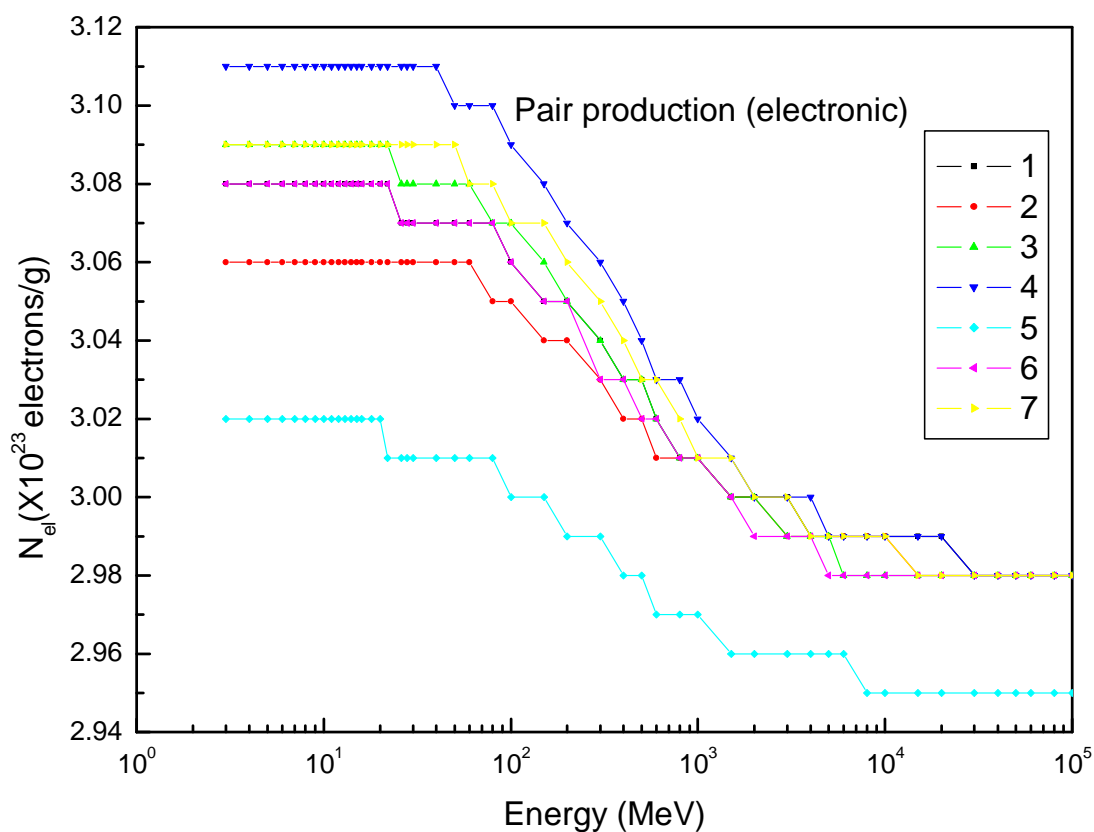


Fig. 13. Variation of effective electron density  $N_{ei}$  of Chemical explosives with photon energy for pair production in electric field.

Table 1 The molecular formula of chemical explosives

S N	Name	Molecular formula
1	Trinitrotoluene (TNT)	$C_7H_5N_3O_6$
2	Trinitrophenylmethylnitramine (Tetryl)	$C_7H_5N_5O_8$
3	Pentaerythritoltetranitrate (PETN)	$C_5H_8N_4O_{12}$
4	Ciklotrimetilentrinitramin (RDX)	$C_3H_6N_3O_6$
5	Picryl chloride (PC)	$C_6H_2ClN_3O_6$
6	Nitroglycerin (NG)	$C_3H_5N_3O_9$
7	Octogene (OG)	$C_4H_8N_8O_8$



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